Simultaneously Solving Computational Problems Using an Artificial Chemical Reactor

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ABSTRACT

This paper is centered on using chemical reaction as a computational metaphor for simultaneously solving problems. An artificial chemical reactor that can simultaneously solve instances of three unrelated problems was created. The reactor is a distributed stochastic algorithm that simulates a chemical universe wherein the molecular species are being represented either by a human genomic contig panel, a Hamiltonian cycle, or an aircraft landing schedule. The chemical universe is governed by reactions that can alter genomic sequences, re-order Hamiltonian cycles, or reschedule an aircraft landing program. Molecular masses were considered as measures of goodness of solutions, and represented radiation hybrid (RH) vector similarities, costs of Hamiltonian cycles, and penalty costs for landing an aircraft before and after target landing times. This method, tested by solving in tandem with deterministic algorithms, has been shown to find quality solutions in finding the minima RH vector similarities of genomic data, minima costs in Hamiltonian cycles of the traveling salesman, and minima costs for landing aircrafts before or after target landing times.

Keywords

Artificial chemical reactor, Traveling salesman problem, Radiation-hybrid mapping, Aircraft landing scheduling

1. INTRODUCTION

Combinatorial optimization problems such as traveling salesman problem (TSP), job-shop scheduling, vehicle routing, scheduling of aircraft landing, gene sequencing, and many others are problems whose solutions are of real-world importance. Exact algorithms have been proposed to these problems but prove inefficient for large problem instances (i.e., they are NP-hard) [17]. Graph-based heuristics such as branch and bound [27], as well as distributed

multi-agent based algorithms such as genetic algorithms [25], memetic algorithms [24, 13, 14], tabu search [28], simulated annealing [22], simulated jumping [3], neural networks [23], and swarm intelligence [15, 16, 11] have been used to find time-restrained optimal and near optimal solutions for these problems.

In recent years, different researchers have shown that the chemical systems of living organisms possess inherent computational properties [18, 1, 4]. Because of these, the chemical metaphor has emerged as a computational paradigm [9, 12, 5, 19, 6, 10]. Under this computational framework, objects such as atoms or molecules are considered as data or solutions, while interactions (i.e., molecular collisions or reactions) among objects are defined by an algorithm.

Using the chemical metaphor, a distributed stochastic algorithm was designed to simulate a reactor where the molecules are being represented either by a human genomic contig panel, a Hamiltonian cycle, or an aircraft landing schedule. The chemical universe in the reactor is governed by reactions that can alter genomic sequences, re-order Hamiltonian cycles, or schedule an aircraft landing program. This computational paradigm can be used to solve, in parallel, very hard real-world problems.

In this effort, an artificial chemical reactor (ACR) simulates chemical catalysis that will solve in parallel three NP-hard computational problems. These problems are the construction and integration of RH map of the human genome, the solution to large instances of symmetric and asymmetric TSP, and the static aircraft landing scheduling problems (ALSP). The artificial chemical reactor was used as a computational metaphor for constructing RH maps from different RH panels and integrating them to produce a single RH map for the genome. The ACR simulation of catalytic reactions constructs RH maps with the same quality as those constructed by RHMAPPER [26] and CONCORDE [2]. In addition, ACR was also used to find, in parallel, solutions to the TSP and the ALSP.

2. DEVELOPMENT OF ARTIFICIAL CHEMICAL REACTOR

This section briefly defines the three problems used in this study: the RH mapping problem, the TSP, and the ALSP. The development of the ACR is then discussed, while its

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underlying reaction algorithms defined, with a focus on solving the three problems in parallel.

2.1 RH Mapping Problem

The RH mapping problem can be viewed as follows. Given a collection of DNA¹ fragments originating from identical copies of a chromosome, where some of the fragments are overlapping while others are disjoint. The problem is to derive the true DNA sequence of the chromosome from these DNA fragments. Since the DNA sequence of the chromosome is unknown, a metric is needed to quantify the correctness of a candidate sequence. A reasonable measure is to find the shortest DNA sequence that has all the fragments as subsequence [20]. This problem is generally known as the shortest common supersequence (SCS).

Given a finite alphabet Σ , where in this case $|\Sigma| = 4$ pertaining to the DNA bases adenine, cytosine, guanine, and thymine, and a finite set of strings R from the superset Σ^* . R can be seen as the set of RH panels. The solution to SCS is a string $w \in \Sigma^*$ such that each string $y \in R$ is a subsequence of w (i.e. one can get y by taking away letters from w) [21]. In RH mapping problem, any string w is a DNA sequence. The minimum length w will be the optimal solution to the RH mapping problem.

2.2 Traveling Salesman Problem

The TSP is formally defined as the problem of finding the shortest Hamiltonian cycle of a graph G(V, E) composed of a set of cities $V = \{v_a, v_2, \ldots, v_n\}$, and a path set $E = \{(v_i, v_j) : v_i, v_j \in V\}$. Associated with G is a cost matrix C where each element $c_{i,j} \in C$ is the cost measure associated with path $(v_i, v_j) \in E$. A Hamiltonian cycle is a closed tour that visits each city $v_i \in V$ once. A symmetric TSP is when $c_{i,j} = c_{j,i}$, otherwise it is an asymmetric TSP. The solution to the TSP is a Hamiltonian tour with the minimum cost f_v (Equation 1).

$$f_v = c_{n,1} + \sum_{i=1}^{n-1} c_{i,i+1}$$
, where $n = \text{number of cities}$ (1)

2.3 Aircraft Landing Scheduling Problem

The ALSP is the problem of deciding a landing time for a set of aircrafts P such that the total penalty cost f_p for landing earlier or later than a target time is minimized. Given, for each aircraft $p_i \in P$ are:

- 1. the earliest landing time e_i ;
- 2. the latest landing time l_i ;
- 3. the target landing time t_i ;
- 4. the penalty cost per unit time, g_i , for landing before t_i ;
- 5. the penalty cost per unit time, h_i , for landing after t_i ;
- 6. the required separation time between p_i landing and p_j landing s_{ij} (where p_i lands before p_j and $p_j \in P$);
- 7. the unknown landing time x_i ; and

8. a dependency variable δ_{ij} , where $\delta_{ij}=1$ if p_i lands before p_j and 0 otherwise.

The ALSP is formally defined in the mathematical programming formulation [7, 8] shown in Equation 2.

$$f_{p} = \sum_{i=1}^{|P|} \{g_{i} \max(0, t_{i} - x_{i}) + h_{i} \max(0, x_{i} - t_{i})\}$$
s.t. $\delta_{ij} + \delta_{ji} = 1, j > i; i, j = 1, \dots, |P|$

$$x_{j} \geq x_{i} + s_{ij}\delta_{ij} - (l_{i} - e_{i})\delta_{ij}, i = j; i, j = 1, \dots, |P|$$

$$e_{i} \leq x_{i} \leq l_{i}, i = 1, \dots, |P|.$$
(2)

2.4 Artificial Chemical Reactor

The artificial chemical reactor (ACR) is defined by a triple ACR(M,R,A). M is a set of artificial molecules, R is a set of reaction rules describing the interaction among molecules, and A is an algorithm driving the reactor. In this paper, the molecules in M are DNA sequences, Hamiltonian tours, or aircraft landing schedules. The rules in R are reordering algorithms that create new molecules when two molecules collide. The algorithm A describes how the rules are applied to a vessel of artificial molecules simulating a well-stirred, topology-less reactor. A partitions the reactor into different levels of reaction activities. The level of reaction activity is a function of molecular mass.

The RH strings $w_i \in \Sigma^*$ ($\forall i = 1, \ldots, |\Sigma^*|$), the set of all permutations $\Pi(V)$ of the |V| cities in V) of the TSP, and the set of all permutations $\Pi(P)$ of the |P| aircrafts in P in the ALSP were considered as molecules. A string w_i encodes a DNA sequence that solves the RH mapping problem, a permutation π_V encodes a Hamiltonian cycle that solves the TSP, and a permutation π_P encodes a landing schedule that solves the ALSP. The width $|w_i|$ of w_i , the cost f_v (Equation 1) of traversing a specific π_V , and the cost f_p (Equation 2) of scheduling a specific π_P were considered as molecular mass.

If two molecules m_1 and m_2 collide and they encode solutions to the same problem, they react following a zero-order catalytic reactions of the form

$$m_1 + m_2 + C \longrightarrow m_3 + m_4$$
,

where m_i are molecules ($\forall i = 1, ..., 4$) and C is a catalyst. The reaction can be mathematically thought of as a function

$$R_1: M \times M \longrightarrow M \times M$$
,

where $m_i \in M$. R_1 performs reordering of solutions as described by the following algorithm (let n be the length of the DNA sequence in the RH mapping problem, or the number of cities in the TSP, or the number of aircrafts in the ALSP – atom is taken as either a DNA base, a city, or an aircraft):

- 1. Let an integer $l \in [1, n]$ be the index of the lth atom in any molecule m. Let i = 1.
- 2. Take a random integer between 1 and n and assign it to l. Let $l^0 = l$.
- 3. Taking the reactant m_i , locate the lth atom and move it as the lth atom for m_{i+2} .

¹deoxyribonucleic acid

- Take note of the lth atom in m_{i+2} and locate it in m_i.
 Replace l with the value of the index of the atom in m_i.
- 5. Repeat steps 3 to 4 until the *l*th atom in m_{i+2} is the same as the l^0 th atom in m_i .
- For all indeces l with no atoms yet in m_{i+2}, move the lth atom from reactant m_i as the lth atom in product m_{i+2}.
- 7. Repeat steps 2 to 6 for i = 2.

If two molecules m_5 and m_6 collide and they encode solutions to different problems, they react following a zero-order catalytic reaction of the form

$$m_5 + m_6 \longrightarrow m_7 + m_8$$
.

The reaction follows a mathematical function

$$R_2: M \times M \longrightarrow M \times M$$

and is described by the following algorithm:

- 1. Let i = 5.
- 2. Take molecule m_i and mark the point of collision as l.
- 3. Take the lth atom in m_i and swap it with the l+1th atom in m_i . If l=n, swap the lth atom with the first atom, instead.
- 4. The resulting molecule is the product m_{i+2}
- 5. Repeat steps 2 to 4 for i = 6.

If a molecule m_9 hits the bottom or walls of the reactor, a zero-order catalytic reaction of the form

$$m_9 + C \longrightarrow m_{10}$$

happens. The reaction is a mathematical function

$$R_3: M \longrightarrow M$$

described by the following algorithm:

- 1. Mark the point of collision in m_9 as l.
- 2. Take the *l*th atom in m_9 and swap it with the l+kth atom. With a probability > 0.5, assign k=1, else k=-1.
- 3. If l = n, swap the lth atom with the first atom instead (for k = 1).
- 4. If l = 1, swap the lth atom with the nth atom instead (for k = -1).

The reactor algorithm A operates on a universe of molecules $S = \{m_1, \ldots, m_{|S|}\}, |S| << |M|$. The development of S is realized by applying the following algorithm:

1. Initialize S with |S| molecules selected randomly from M.

- Using stochastic sampling with replacement, select two molecules m₁ and m₂ from S without removing them.
- 3. Apply the reaction rule R_1 if m_1 and m_2 encode solutions to the same problem. Otherwise, apply R_2 instead to get the products m_3 and m_4 .
- 4. Apply the reaction rule R_3 for heavy molecules that collide with the reactor walls and bottom.
- Decay the heavier molecules by removing them out of S
 and replacing them with randomly selected molecules
 from M.
- Repeat steps 2 to 5 until S is saturated with lighter molecules.

One iteration of A constitutes one epoch in the artificial reactor. The sampling procedure gives molecules with low molecular mass a higher probability to react or collide with other molecules. This mimics the level of excitation energy the molecule needs to overcome for it to react with another molecule. This means that the lighter the molecule, the higher the chance that it will collide with other molecules. Step 6 of algorithm A requires a metric for measuring saturation of molecules. In this study, when the number of molecules in that level of excitation has reached 90% of the total molecules encoding the same problem, the ACR will stop applying the reaction rules for the same problem and will consider it solved while continuing the simulation for the remaining problems.

3. RESULTS AND DISCUSSION

Using the same datasets and parameters from results on recently published papers on RH mapping [2], TSP [16], and ALSP [8], the ACR was run to solve the three problems in parallel. A single-processor Pentium IV machine with 1.2GHz bus speed running under a multiprogramming operating system was used to run the ACR simulations. The ACR simulation was repeated 10 times while each of the problem's metrics (i.e., the best minimum for each run) were recorded. The values recorded were averaged and the standard deviation computed. The results of the runs were compared to those of the recent literature. The comparison are summarized in tables.

3.1 RH Mapping

Tables 1 and 2 show the average obligate chromosome breaks per marker for the GB4 and G3 RH panels, respectively, as found by RHMAPPER and CONCORDE (both reported by [2]) and ACR. The tables show the averages of 10 runs for each chromosome for ACR and the respective standard deviations. The tables show that the result found by ACR is not different from the results found by either RHMAPPER or CONCORDE.

3.2 Symmetric and Asymmetric TSPs

Table 3 compares the average tour lengths found by ACR, simulated annealing, and self-organizing maps on five sets of random instances of symmetric 50-city TSPs. The table shows the average value of 10 runs for ACR and the respective standard deviation. Table 4, on the other hand, compares the best integer tour length found by ACR and genetic

Table 1: The average obligate chromosome breaks per marker for the GB4 panel as found by RHMAPPER, CONCORDE and ACR. The ACR values are averaged over 10 runs while the values in parenthesis are the respective standard deviation.

parenthesis are the respective standard deviation.				parenth
Chromosome	RHMAPPER	CONCORDE	ACR	Chromo
Number			(std. dev.)	Num
1	-	1.66	1.88 (0.20)	1
2	3.80	2.12	2.56 (0.64)	2
3	2.71	1.97	1.80 (0.85)	3
4	3.75	2.15	3.22(0.55)	4
5	3.37	1.99	2.67(0.38)	5
6	2.60	1.70	2.60(0.80)	6
7	2.86	1.92	1.88(0.90)	7
8	3.64	2.09	2.88(0.47)	8
9	2.86	1.85	2.88(0.99)	9
10	3.55	2.04	1.99(0.55)	10
11	2.53	1.86	1.95 (0.64)	11
12	3.87	1.98	3.27 (0.85)	12
13	2.92	2.01	2.46 (0.85)	13
14	2.43	1.79	2.15 (0.59)	14
15	4.16	2.25	3.00(0.88)	15
16	3.18	2.32	2.74(0.78)	16
17	2.74	2.03	2.00(0.67)	17
18	3.07	2.47	2.20(0.83)	18
19	2.78	1.99	2.66(0.74)	19
20	2.41	1.74	2.50 (0.70)	20
21	2.64	2.19	2.33(0.41)	21
22	2.87	2.17	2.33(0.64)	22
23	2.36	1.70	2.36 (0.66)	23

the ACR will suffer considerably in terms of efficiency. Thus, further investigations on the use of multi-processor machines are needed to achieve better ACR performance.

algorithm on four examples of asymmetric instances of TSP. Based on the data presented in both tables, it can be seen that ACR's performance is similar to the performances of the other search techniques employed by other researchers.

3.3 Scheduling Aircraft Landings

Table 5 shows the performance of ACR as compared to the optimal solutions of eight instances of aircraft landing problems. From the data presented, it can be seen that ACR was able to find near optimal solutions for six out of eight problems, and the exact solution for two out of eight problems.

4. CONCLUDING REMARKS

An ACR that mimicked catalytic reactions was designed to simultaneously solve three unrelated problems. The catalytic reactions of the ACR were able to construct RH maps with similar qualities found by deterministic algorithms. In addition, ACR was found to be applicable in finding solutions to TSPs and ALSPs in parallel with RH mapping. Thus, ACR may be used to simultaneously solve hard problems such as the RH mapping, TSP, and ALSP.

The work described in this paper can be extended as follows. In order to assess its efficiency, additional experiments are needed with the ACR simulating more than three problems simultaneously. This experiment will answer the question: "Up to how many problems will the ACR be still efficient?" Using a single-processor machine, as the number of problems being solved simultaneously is increased, it is expected that

Table 2: The average obligate chromosome breaks per marker for the G3 panel as found by RHMAPPER, CONCORDE and ACR. The ACR values are averaged over 10 runs while the values in parenthesis are the respective standard deviation.

-			
Chromosome	RHMAPPER	CONCORDE	ACR
Number			(std. dev.)
1	-	2.91	2.88 (0.06)
2	4.96	2.88	2.92(0.02)
3	5.18	3.13	2.10(0.03)
4	5.52	2.96	4.21(0.47)
5	5.17	3.09	3.52(0.98)
6	4.76	3.11	2.66(0.01)
7	5.91	3.69	2.25(0.65)
8	5.34	3.09	3.36(0.22)
9	4.73	3.16	3.33(0.55)
10	5.35	3.47	2.81(0.54)
11	5.79	3.24	2.70(0.06)
12	5.31	3.32	3.60(0.90)
13	4.58	3.17	2.86(0.69)
14	4.04	2.93	2.81(0.20)
15	4.70	3.76	3.19(0.50)
16	5.04	3.49	2.75(0.26)
17	4.39	3.69	2.01(0.32)
18	6.10	3.88	2.49(0.56)
19	4.95	3.23	2.82(0.10)
20	4.87	3.70	3.15(0.65)
21	3.79	3.36	2.42 (0.32)
22	4.21	3.41	3.31 (0.88)
23	4.35	2.80	2.84 (0.47)
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Table 3: Comparison of average tour length found by ACR, simulated annealing (SA), and self-organizing maps (SOM) on five sets of random instances of symmetric 50–city TSPs. ACR values are averaged over 10 runs. The values in parenthesis are the standard deviation of the 10 runs for ACR.

Problem	ACR (std. dev.)	SA	SOM
1	5.87(0.33)	5.88	6.06
2	6.15 (0.08)	6.01	6.25
3	5.59(0.21)	5.65	5.83
4	5.67(0.98)	5.81	5.87
5	6.15 (0.54)	6.33	6.70

Table 4: Comparison of the best integer tour length found by ACR and genetic algorithm (GA) on four examples of asymmetric instances of TSPs.

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Problem	ACR	GA	
Oliver 30	421	421	
Ei150	424	428	
Ei175	550	545	
Krot100	21,280	21,761	

Table 5: Comparison between the optimal cost of scheduling aircraft landings and those found by ACR on eight instances of ALSP.

Problem	Number of	Number of	Optimal	ACR
Number	Aircrafts	Runways	Solution	
1	10	1	700	721
2	10	2	90	94
3	20	1	1,480	1,463
4	20	2	210	220
5	30	1	24,442	24,536
6	30	2	554	554
7	50	1	1,950	2,001
8	50	2	135	135

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